Tom K Woo

List of Publications by Year
in descending order

47 papers	4,393 citations	218677 26 h-index	233421 45 g-index
49 all docs	49 docs citations	49 times ranked	4797 citing authors

#	Article	IF	Citations
1	Inverse design of nanoporous crystalline reticular materials with deep generative models. Nature Machine Intelligence, 2021, 3, 76-86.	16.0	172
2	A scalable metal-organic framework as a durable physisorbent for carbon dioxide capture. Science, 2021, 374, 1464-1469.	12.6	308
3	Molecular dynamics simulations of interfacial properties of the CO2â€“water and CO2â€“CH4â€“water systems. Journal of Chemical Physics, 2020, 153, 044701.	3.0	18
4	High-Performing Deep Learning Regression Models for Predicting Low-Pressure CO₂ Adsorption Properties of Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2020, 124, 27996-28005.	3.1	39
5	An Ultraâ€Microporous Metalâ€“Organic Framework with Exceptional Xe Capacity. Chemistry - A European Journal, 2020, 26, 12544-12548.	3.3	10
6	Prediction of MOF Performance in Vacuum Swing Adsorption Systems for Postcombustion CO₂ Capture Based on Integrated Molecular Simulations, Process Optimizations, and Machine Learning Models. Environmental Science & Technology, 2020, 54, 4536-4544.	10.0	117
7	Molecular Dynamic Simulations of Clathrate Hydrate Anomalous Preservation: The Effect of Coating Clathrate Hydrate Phases. Journal of Physical Chemistry C, 2019, 123, 28715-28725.	3.1	9
8	Design Strategy for the Controlled Generation of Cationic Frameworks and Ensuing Anion-Exchange Capabilities. ACS Applied Materials & Interfaces, 2019, 11, 3181-3188.	8.0	11
9	Robust Machine Learning Models for Predicting High CO₂ Working Capacity and CO₂/H₂ Selectivity of Gas Adsorption in Metal Organic Frameworks for Precombustion Carbon Capture. Journal of Physical Chemistry C, 2019, 123, 4133-4139.	3.1	102
10	Imparting gas selective and pressure dependent porosity into a non-porous solid via coordination flexibility. Materials Horizons, 2019, 6, 1883-1891.	12.2	17
11	Interfacial properties of hydrocarbon/water systems predicted by molecular dynamic simulations. Journal of Chemical Physics, 2019, 150, 114703.	3.0	29
12	Data-driven design of metalâ€“organic frameworks for wet flue gas CO2 capture. Nature, 2019, 576, 253-256.	27.8	438
13	Idealized Carbon-Based Materials Exhibiting Record Deliverable Capacities for Vehicular Methane Storage. Journal of Physical Chemistry C, 2019, 123, 1050-1058.	3.1	11
14	Bond Type Restricted Property Weighted Radial Distribution Functions for Accurate Machine Learning Prediction of Atomization Energies. Journal of Chemical Theory and Computation, 2018, 14, 5229-5237.	5.3	2
15	Ultralow Parasitic Energy for Postcombustion CO₂ Capture Realized in a Nickel Isonicotinate Metalâ€“Organic Framework with Excellent Moisture Stability. Journal of the American Chemical Society, 2017, 139, 1734-1737.	13.7	121
16	Stepwise crystallographic visualization of dynamic guest binding in a nanoporous framework. Chemical Science, 2017, 8, 3171-3177.	7.4	66
17	A New Split Charge Equilibration Model and REPEAT Electrostatic Potential Fitted Charges for Periodic Frameworks with a Net Charge. Journal of Chemical Theory and Computation, 2017, 13, 2858-2869.	5.3	12
18	Split-Charge Equilibration Parameters for Generating Rapid Partial Atomic Charges in Metalâ€“Organic Frameworks and Porous Polymer Networks for High-Throughput Screening. Journal of Physical Chemistry C, 2017, 121, 903-910.	3.1	12

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19	Computational and Experimental Assessment of CO₂ Uptake in Phosphonate Monoester Metalâ€“Organic Frameworks. Chemistry of Materials, 2017, 29, 10469-10477.	6.7	17
20	Quantitative Structureâ€“Property Relationship Models for Recognizing Metal Organic Frameworks (MOFs) with High CO₂ Working Capacity and CO₂/CH₄ Selectivity for Methane Purification. European Journal of Inorganic Chemistry, 2016, 2016, 4505-4511.	2.0	68
21	Molecular simulations and density functional theory calculations of bromine in clathrate hydrate phases. Journal of Chemical Physics, 2016, 144, 044501.	3.0	13
22	Materials design by evolutionary optimization of functional groups in metal-organic frameworks. Science Advances, 2016, 2, e1600954.	10.3	82
23	Lowâ€Overpotential Electrocatalytic Water Splitting with Nobleâ€Metalâ€Free Nanoparticles Supported in a sp³ Nâ€Rich Flexible COF. Advanced Energy Materials, 2016, 6, 1600110.	19.5	121
24	A generalized method for constructing hypothetical nanoporous materials of any net topology from graph theory. CrystEngComm, 2016, 18, 3777-3792.	2.6	104
25	Ethanol Electro-oxidation on Palladium Revisited Using Polarization Modulation Infrared Reflection Absorption Spectroscopy (PM-IRRAS) and Density Functional Theory (DFT): Why Is It Difficult To Break the Câ€“C Bond?. ACS Catalysis, 2016, 6, 4894-4906.	11.2	109
26	Intercalation of Coordinatively Unsaturated Fe^{III} Ion within Interpenetrated Metalâ€“Organic Framework MOFâ€5. Chemistry - A European Journal, 2016, 22, 7711-7715.	3.3	15
27	Evaluation of carbon nanoscroll materials for post-combustion CO2 capture. Carbon, 2016, 101, 218-225.	10.3	31
28	A single-ligand ultra-microporous MOF for precombustion CO ₂ capture and hydrogen purification. Science Advances, 2015, 1, e1500421.	10.3	127
29	Molecular dynamics simulation of halogen bonding in Cl₂, BrCl, and mixed Cl₂/Br₂ clathrate hydrates. Canadian Journal of Chemistry, 2015, 93, 864-873.	1.1	15
30	Rapid and Accurate Machine Learning Recognition of High Performing Metal Organic Frameworks for CO₂ Capture. Journal of Physical Chemistry Letters, 2014, 5, 3056-3060.	4.6	234
31	Computational prediction of temperature dependence of 13C NMR lineshapes of planar molecules in structure I clathrate hydrates. Journal of the Iranian Chemical Society, 2013, 10, 659-667.	2.2	2
32	Fast and Accurate Electrostatics in Metal Organic Frameworks with a Robust Charge Equilibration Parameterization for High-Throughput Virtual Screening of Gas Adsorption. Journal of Physical Chemistry Letters, 2013, 4, 3056-3061.	4.6	90
33	Large-Scale Quantitative Structureâ€“Property Relationship (QSPR) Analysis of Methane Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 7681-7689.	3.1	174
34	Atomic Property Weighted Radial Distribution Functions Descriptors of Metalâ€“Organic Frameworks for the Prediction of Gas Uptake Capacity. Journal of Physical Chemistry C, 2013, 117, 14095-14105.	3.1	113
35	Ab initio based large-scale screening of hypothetical MOFs for carbon capture application. Materials Research Society Symposia Proceedings, 2013, 1523, 0301.	0.1	0
36	MOFIA: a chemoinformatic webserver for the prediction of CO2 adsorption in metal organic frameworks (MOF). Materials Research Society Symposia Proceedings, 2013, 1523, 801.	0.1	0

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37	Characterization of Znâ€Containing Metalâ€“Organic Frameworks by Solidâ€State ⁶⁷Zn NMR Spectroscopy and Computational Modeling. Chemistry - A European Journal, 2012, 18, 12251-12259.	3.3	66
38	Back Cover: Characterization of Zn-Containing Metal-Organic Frameworks by Solid-State67Zn NMR Spectroscopy and Computational Modeling (Chem. Eur. J. 39/2012). Chemistry - A European Journal, 2012, 18, 12532-12532.	3.3	0
39	Competition and Cooperativity in Carbon Dioxide Sorption by Amineâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 1826-1829.	13.8	131
40	Phosphonate Monoesters as Carboxylate-like Linkers for Metal Organic Frameworks. Journal of the American Chemical Society, 2011, 133, 20048-20051.	13.7	85
41	Metastable polymeric nitrogen nanotube from a zigzag sheet phase and first-principles calculations. Physical Review B, 2010, 82, .	3.2	11
42	Grand-Canonical Monte Carlo and Molecular-Dynamics Simulations of Carbon-Dioxide and Carbon-Monoxide Adsorption in Zeolitic Imidazolate Framework Materials. Journal of Physical Chemistry C, 2010, 114, 2171-2178.	3.1	83
43	Direct Observation and Quantification of CO ₂ Binding Within an Amine-Functionalized Nanoporous Solid. Science, 2010, 330, 650-653.	12.6	860
44	Genetic algorithm and first-principles DFT study of the high-pressure molecularÎ¶phase of nitrogen. Physical Review B, 2009, 80, .	3.2	13
45	A Computational Experiment of the Endo versus Exo Preference in a Dielsâ€“Alder Reaction. Journal of Chemical Education, 2009, 86, 199.	2.3	22
46	Electrostatic Potential Derived Atomic Charges for Periodic Systems Using a Modified Error Functional. Journal of Chemical Theory and Computation, 2009, 5, 2866-2878.	5.3	281
47	How Do We Simulate Things at the Scale of Molecules and Electrons? An Introduction to the Technology and HPC Aspects of Computational Chemistry. 2008 22nd International Symposium on High Performance Computing Systems and Applications, 2008, , .	0.0	0